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Modelling of the configurations of chain molecules of biopolymers

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Abstract

A method is proposed for the modelling of the configurations of the chain molecules of biopolymers on the basis of their different physicochemical properties. The search for the most suitable model is made in several steps. At first, all the possible modes of passage of the chain modelling the secondary structure of protein through points regularly arranged in volume are considered. From the configurations obtained the authors select those which regularly fill the volume. For the remaining configurations they also calculate such parameters which may be found experimentally for the modelled protein. The method of mathematical logic is used to select from the entire set of configurations those which best meet all the available experimental findings. Probability calculations for the models are made. The method described was used to construct a model of myoglobin and to compare it with the known structure for this protein. As a result, satisfactory reflexion by the model of the location of certain polypeptide chains and their zones was noted. © 1971.